



Valkenier, H., Dias, C. M., Butts, C. P., & Davis, A. P. (2017). A folding decalin tetra-urea for transmembrane anion transport. *Tetrahedron*, 73(33), 4955-4962.
<https://doi.org/10.1016/j.tet.2017.04.064>

Peer reviewed version

License (if available):
CC BY-NC-ND

Link to published version (if available):
[10.1016/j.tet.2017.04.064](https://doi.org/10.1016/j.tet.2017.04.064)

[Link to publication record in Explore Bristol Research](#)
PDF-document

This is the author accepted manuscript (AAM). The final published version (version of record) is available online via Elsevier at <http://www.sciencedirect.com/science/article/pii/S0040402017304659>. Please refer to any applicable terms of use of the publisher.

University of Bristol - Explore Bristol Research

General rights

This document is made available in accordance with publisher policies. Please cite only the published version using the reference above. Full terms of use are available:
<http://www.bristol.ac.uk/red/research-policy/pure/user-guides/ebr-terms/>

Electronic Supplementary Information

for

A folding decalin tetra-urea for transmembrane anion transport

Hennie Valkenier,^{a,b*} Christopher M. Dias,^a Craig P. Butts,^a Anthony P. Davis^{a*}

a. School of Chemistry, University of Bristol, Cantock's Close, Bristol BS8 1TS, United Kingdom.

b. Engineering of Molecular NanoSystems, Ecole Polytechnique de Bruxelles, Université Libre de Bruxelles, Avenue F.D. Roosevelt 50, CP165/64, B-1050 Brussels, Belgium.

** Corresponding authors. Tel: +44117-9546334, Fax: +44117-9251295,
E-mail: Anthony.Davis@bristol.ac.uk, Hennie.Valkenier@ulb.ac.be.*

1. NMR spectra of amine **8**

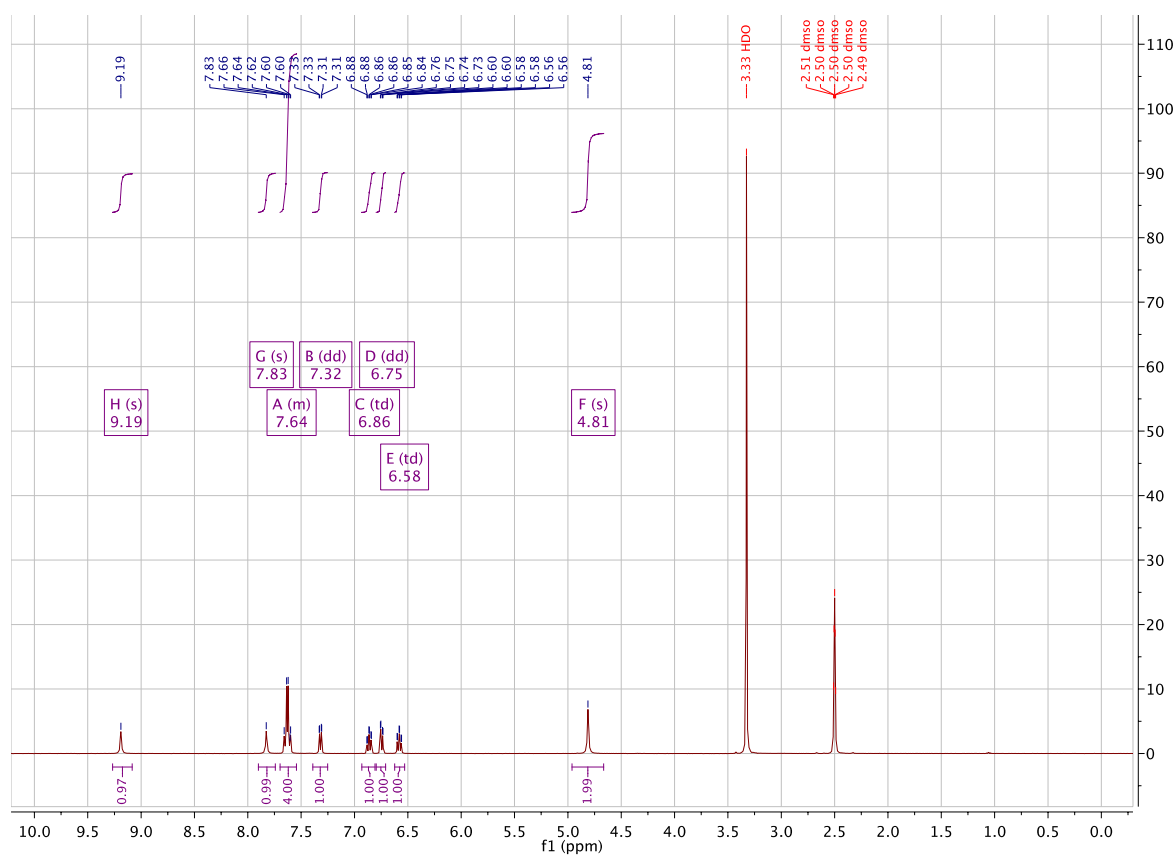


Figure S1. ¹H NMR spectrum of amine **8** in DMSO-d₆ (400 MHz).

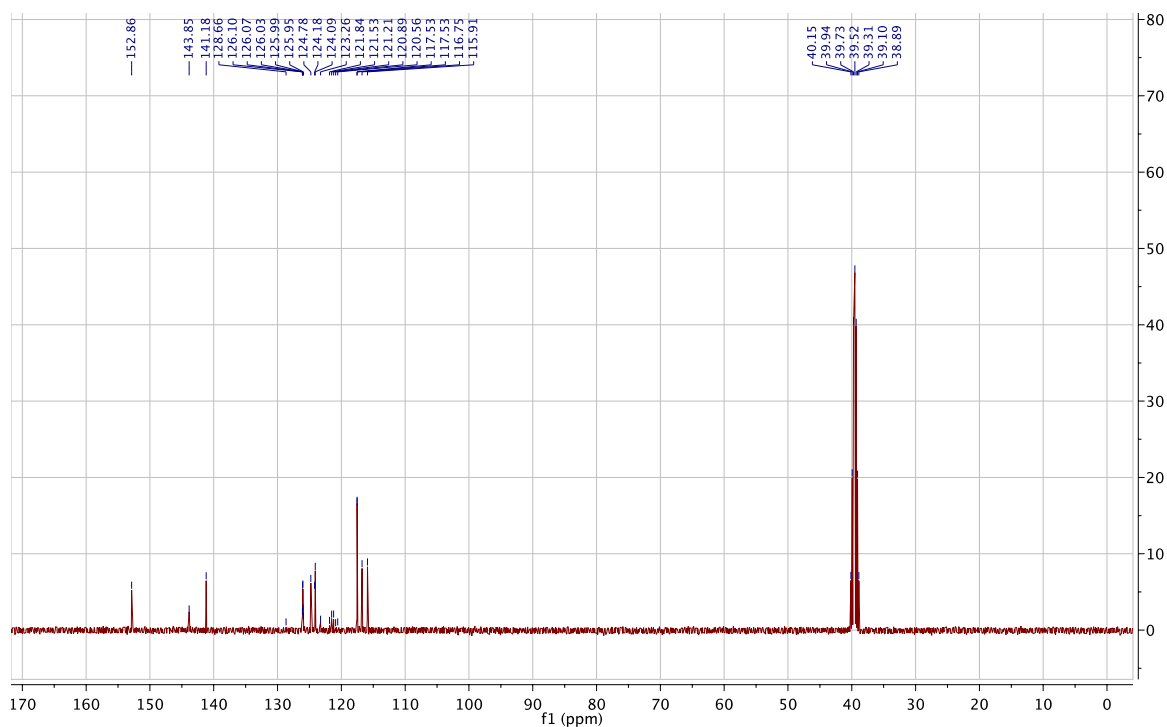


Figure S2. ¹³C NMR spectrum of amine **8** in DMSO-d₆ (101 MHz).

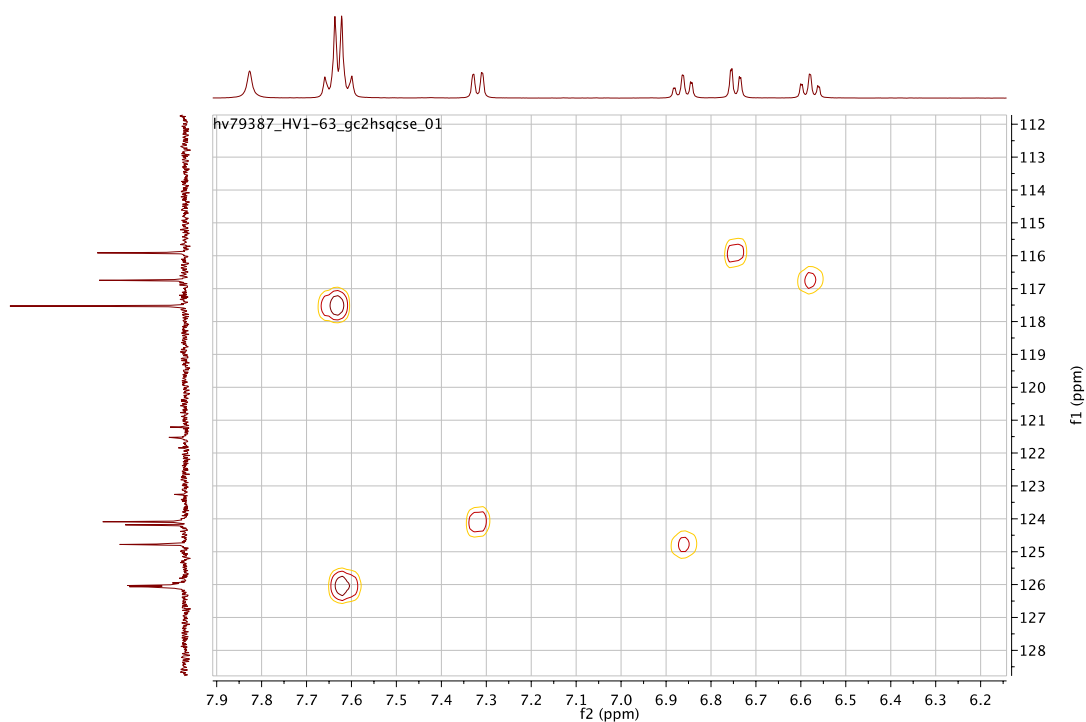


Figure S3. HSQC spectrum of amine **8** in DMSO-d₆ (400 MHz).

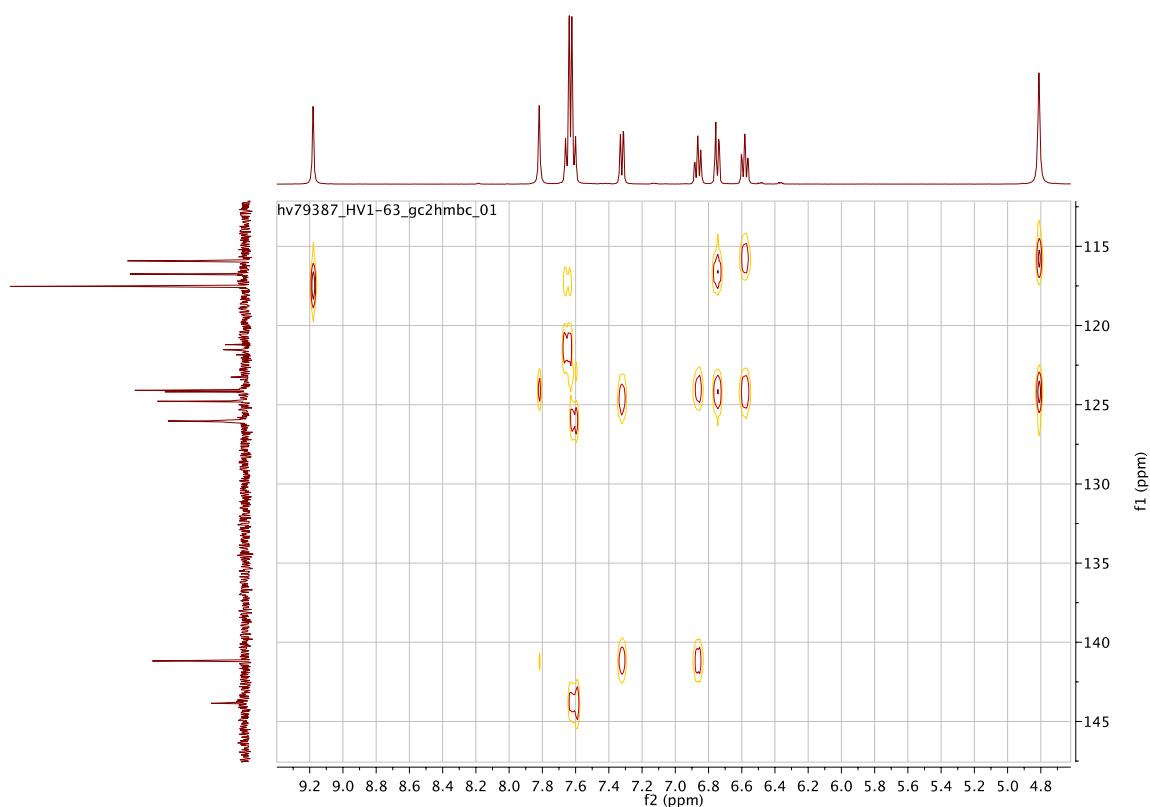


Figure S4. HMBC spectrum of amine **8** in DMSO-d₆ (400 MHz).

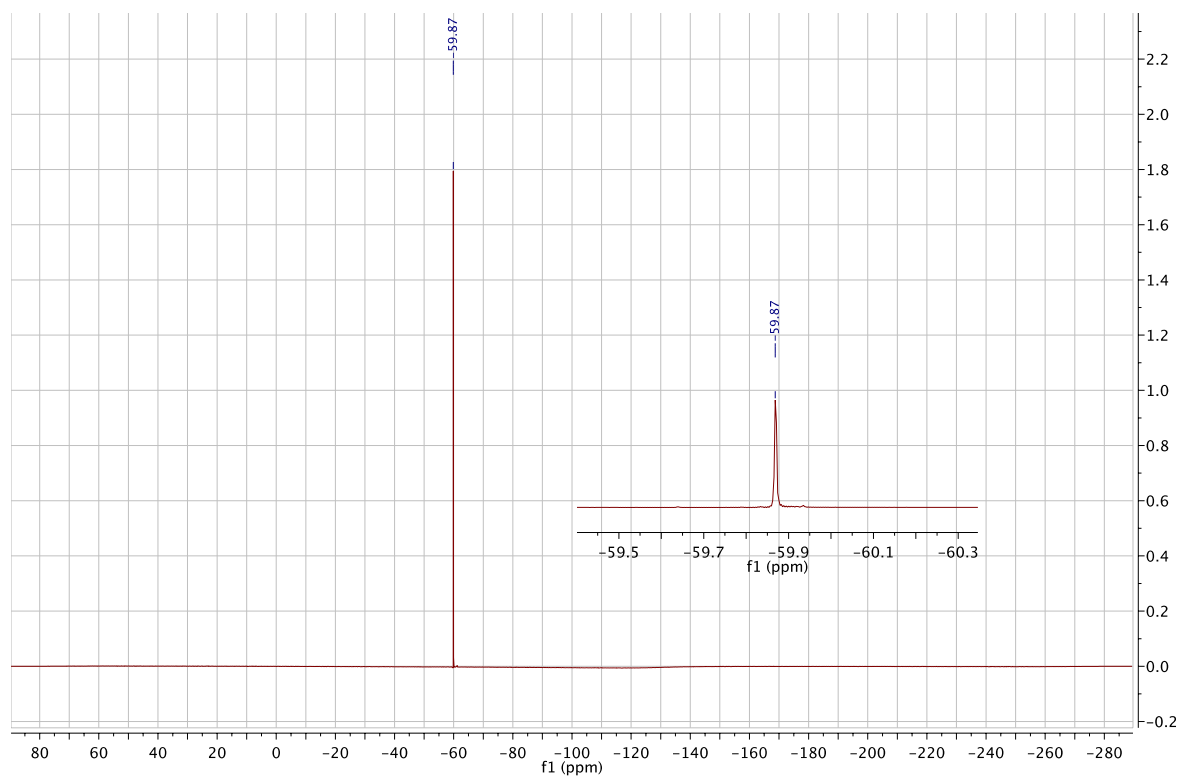


Figure S5. ^{19}F spectrum of amine **8** in DMSO-d_6 (377 MHz).

2. NMR spectra of decalin tetra-urea **7**

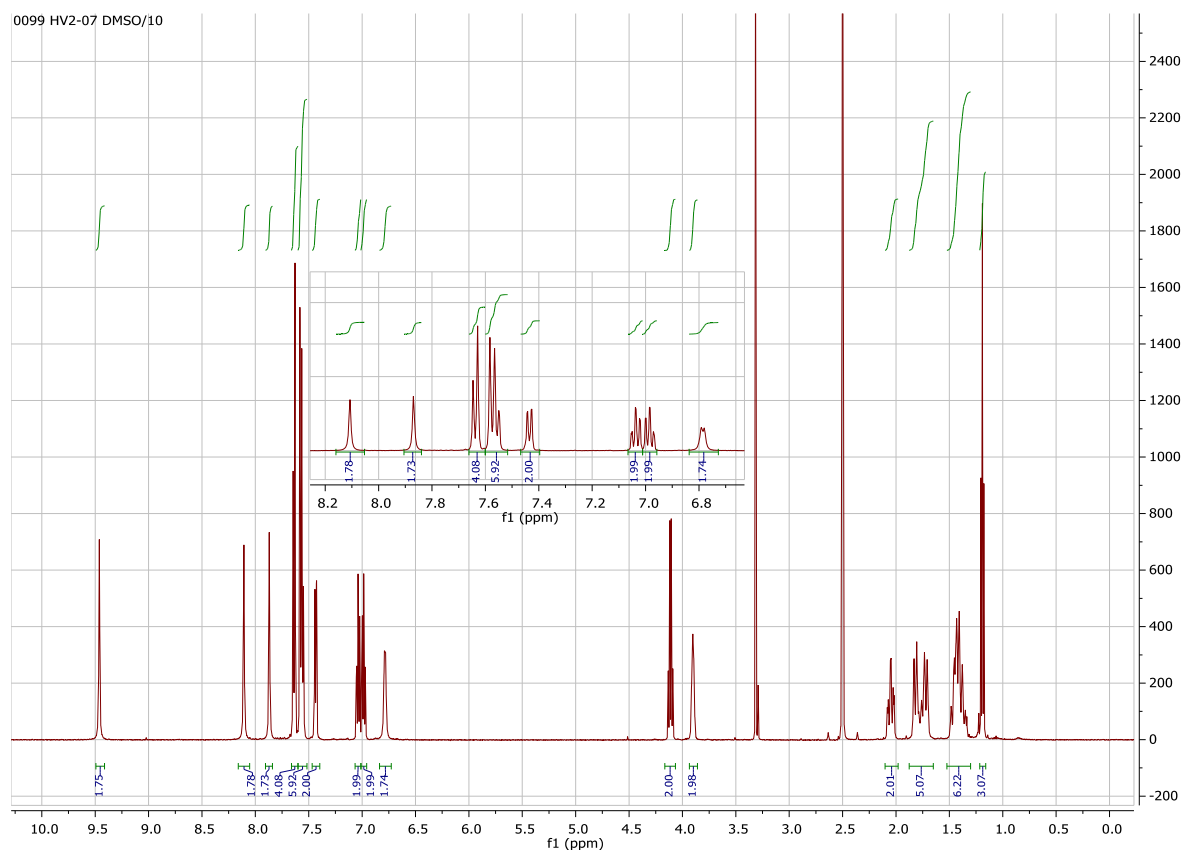


Figure S6. ^1H NMR spectrum of **7** in DMSO- d_6 (500 MHz).

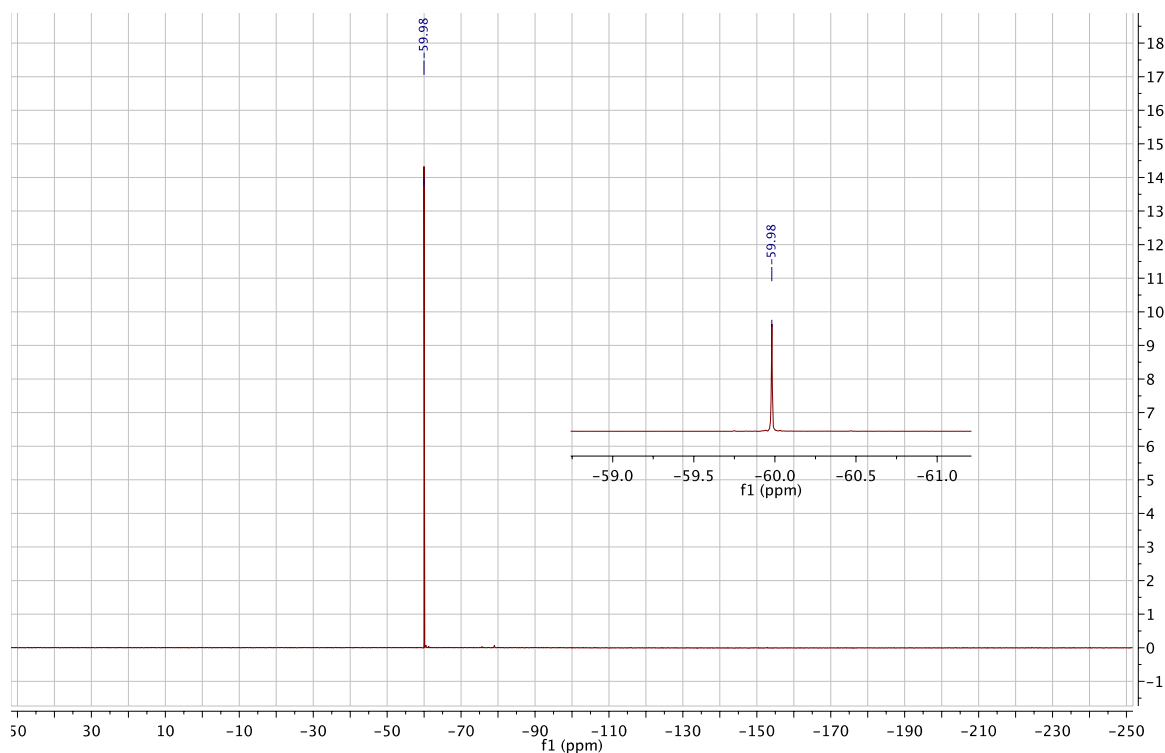


Figure S7. ^{19}F spectrum of **7** in DMSO- d_6 (377 MHz).

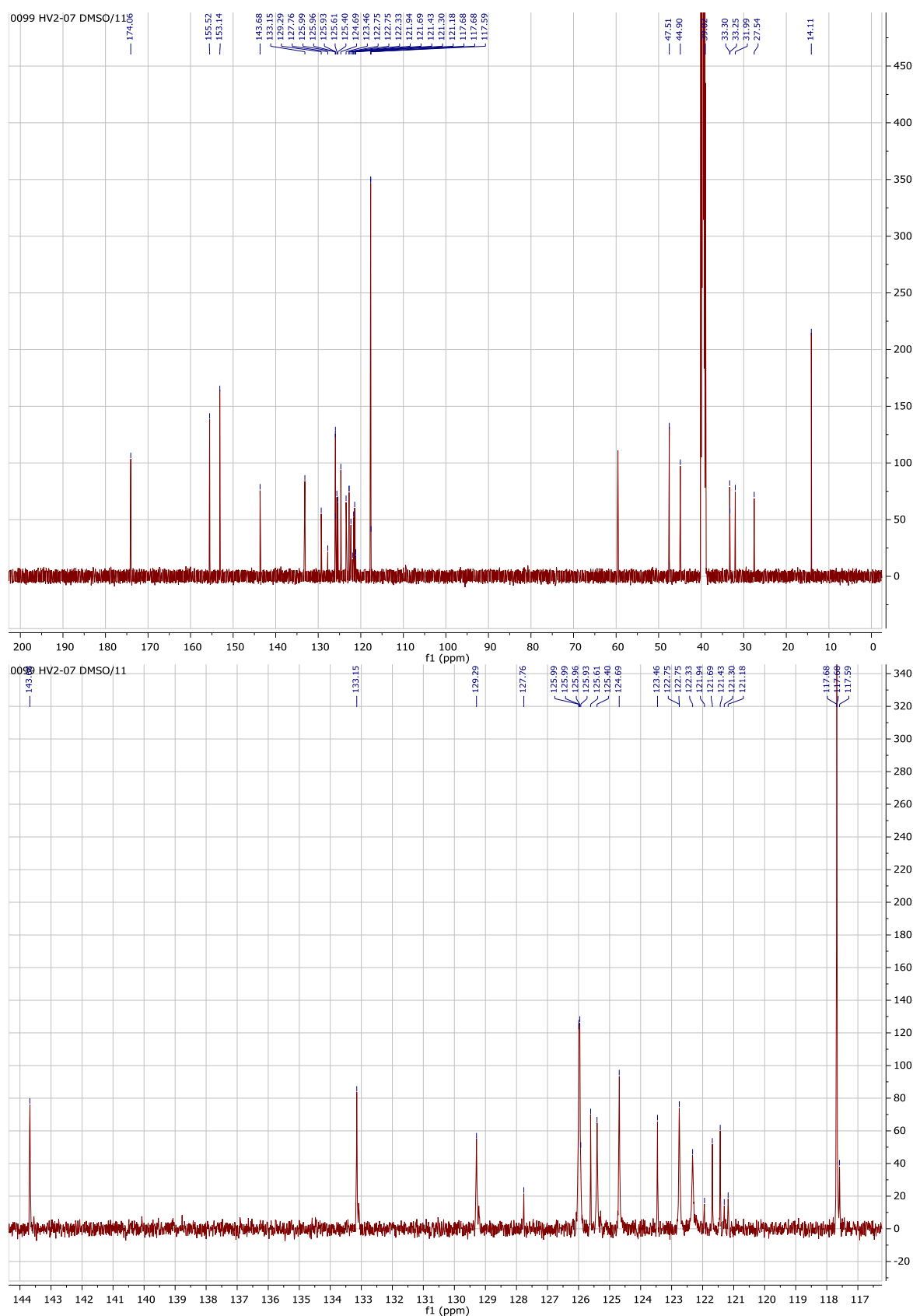


Figure S8. ^{13}C NMR spectra of **7** in DMSO- d_6 (126 MHz).

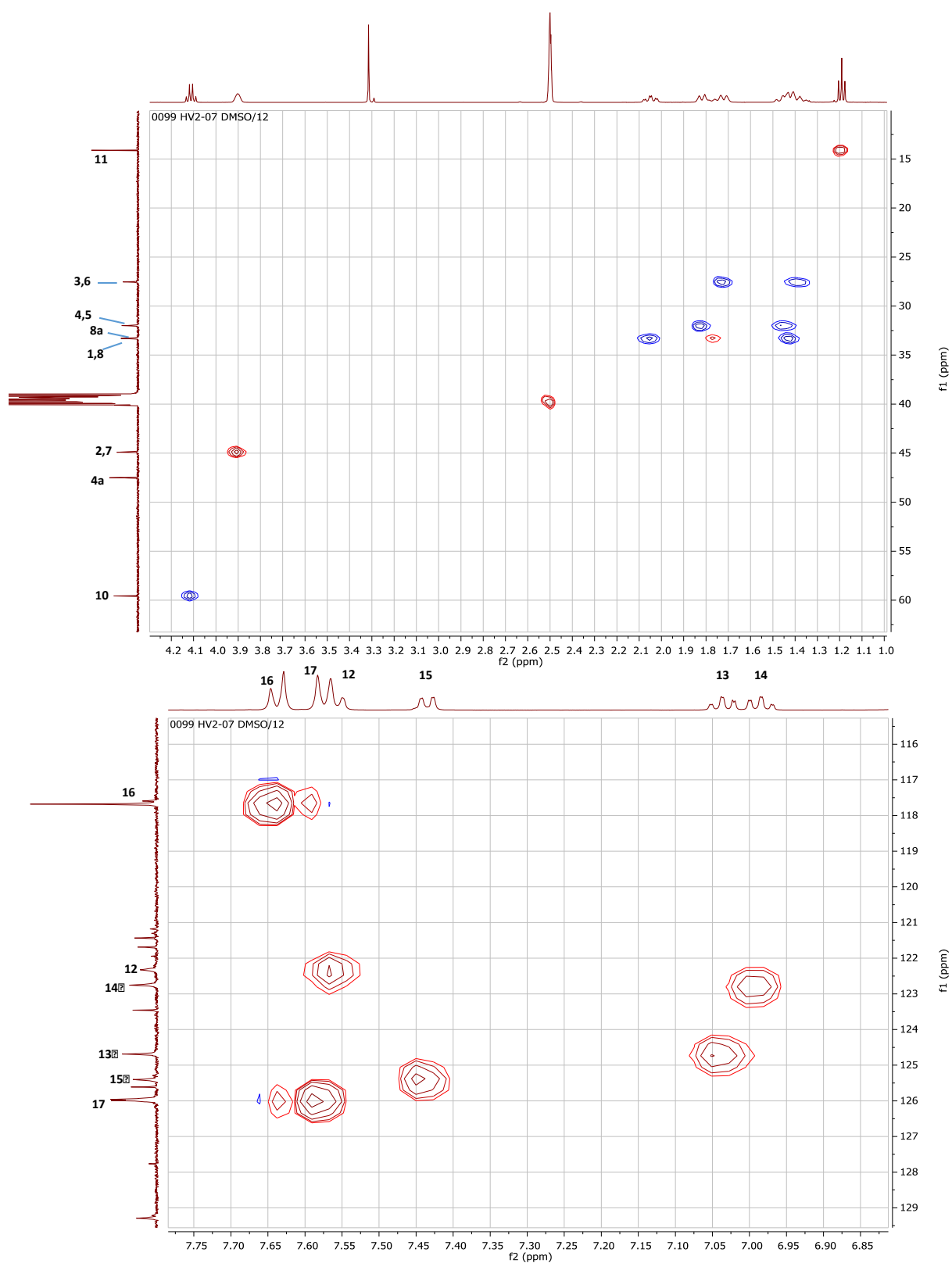


Figure S9. HSQC spectra of **7** in DMSO- d_6 (500 MHz).

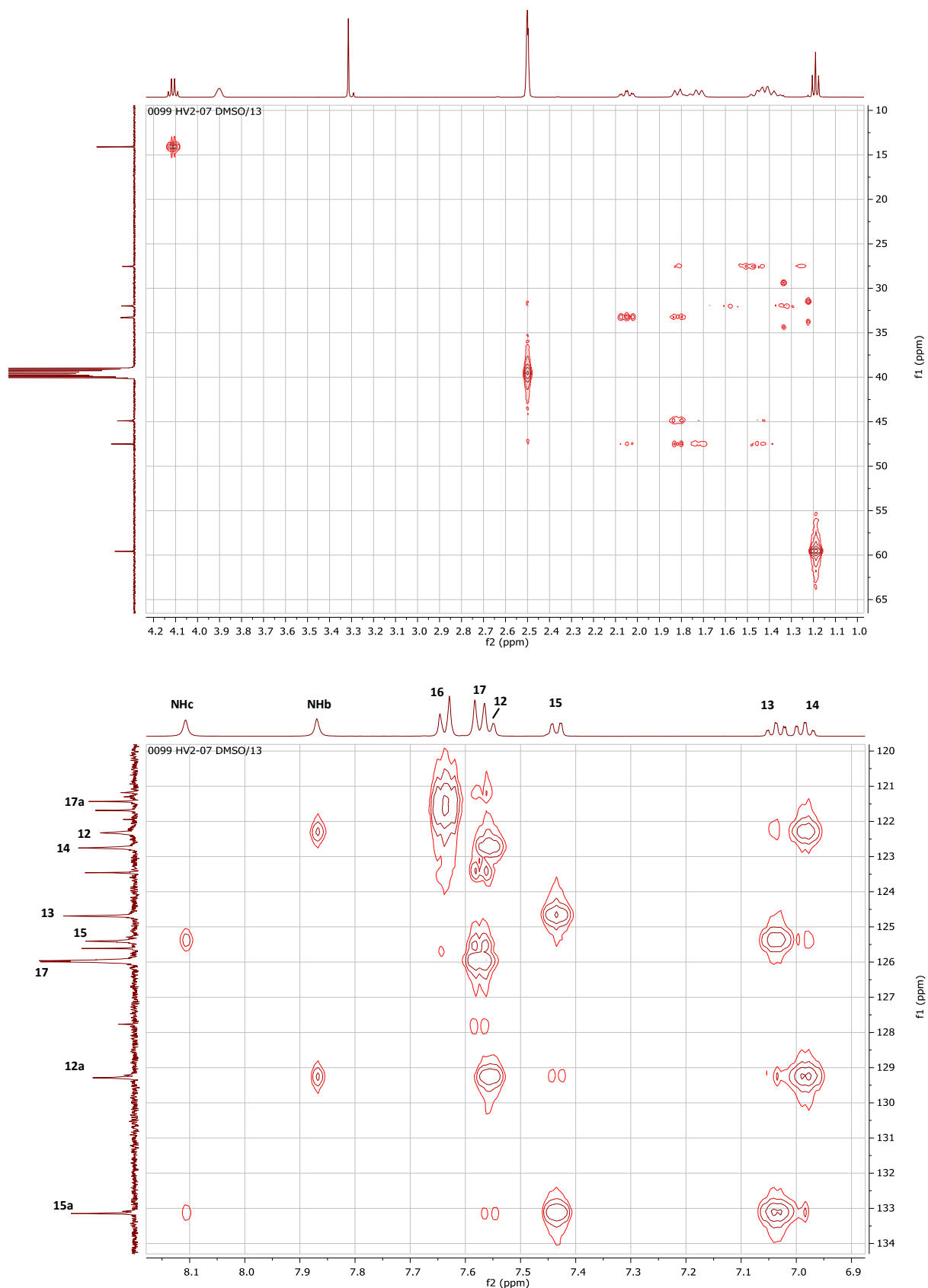


Figure S10. HMBC spectra of **7** in DMSO- d_6 (500 MHz).

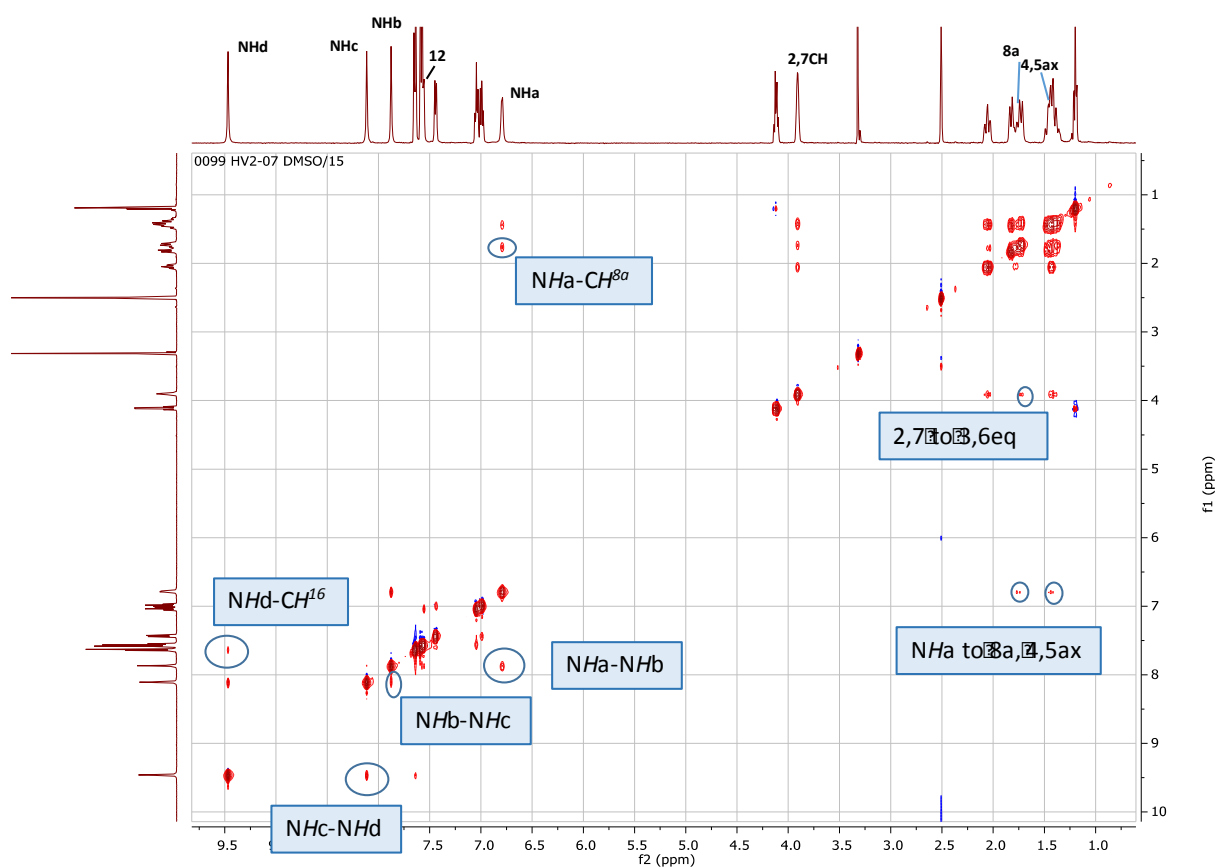


Figure S11. 2D NOESY spectrum of **7** in DMSO- d_6 (500 MHz).

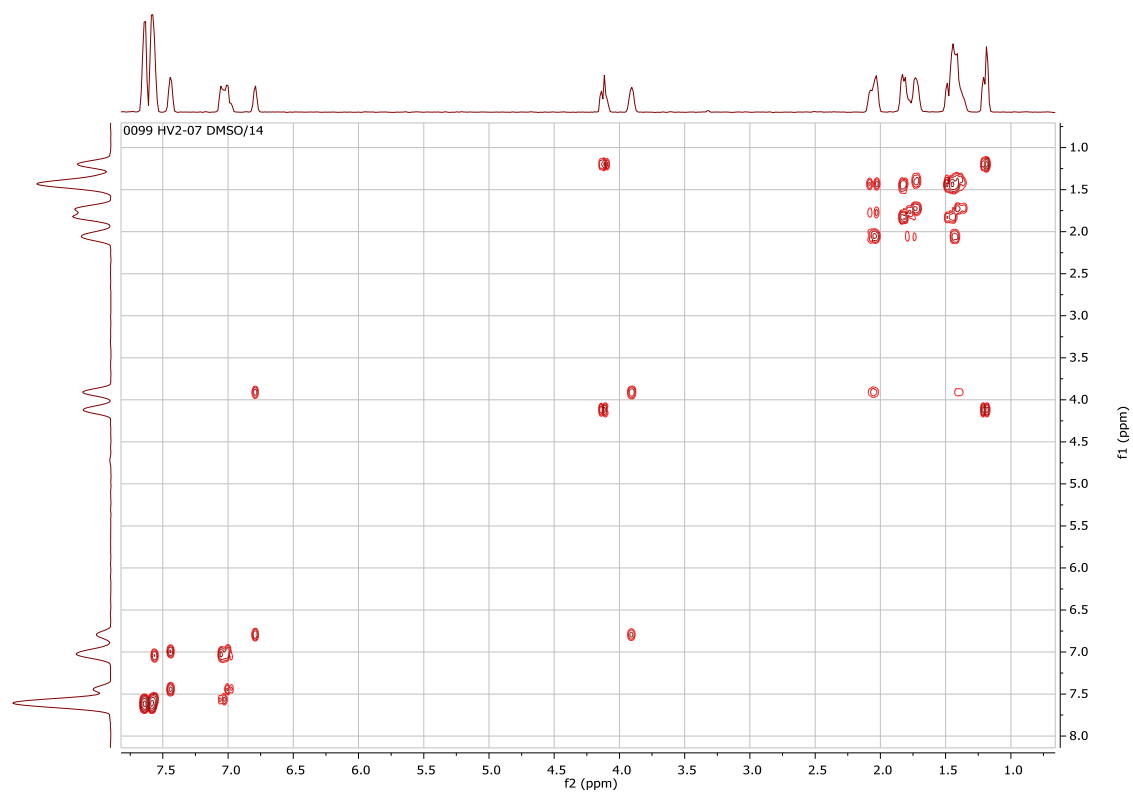


Figure S12. 2D COSY spectrum of **7** in DMSO- d_6 (500 MHz).

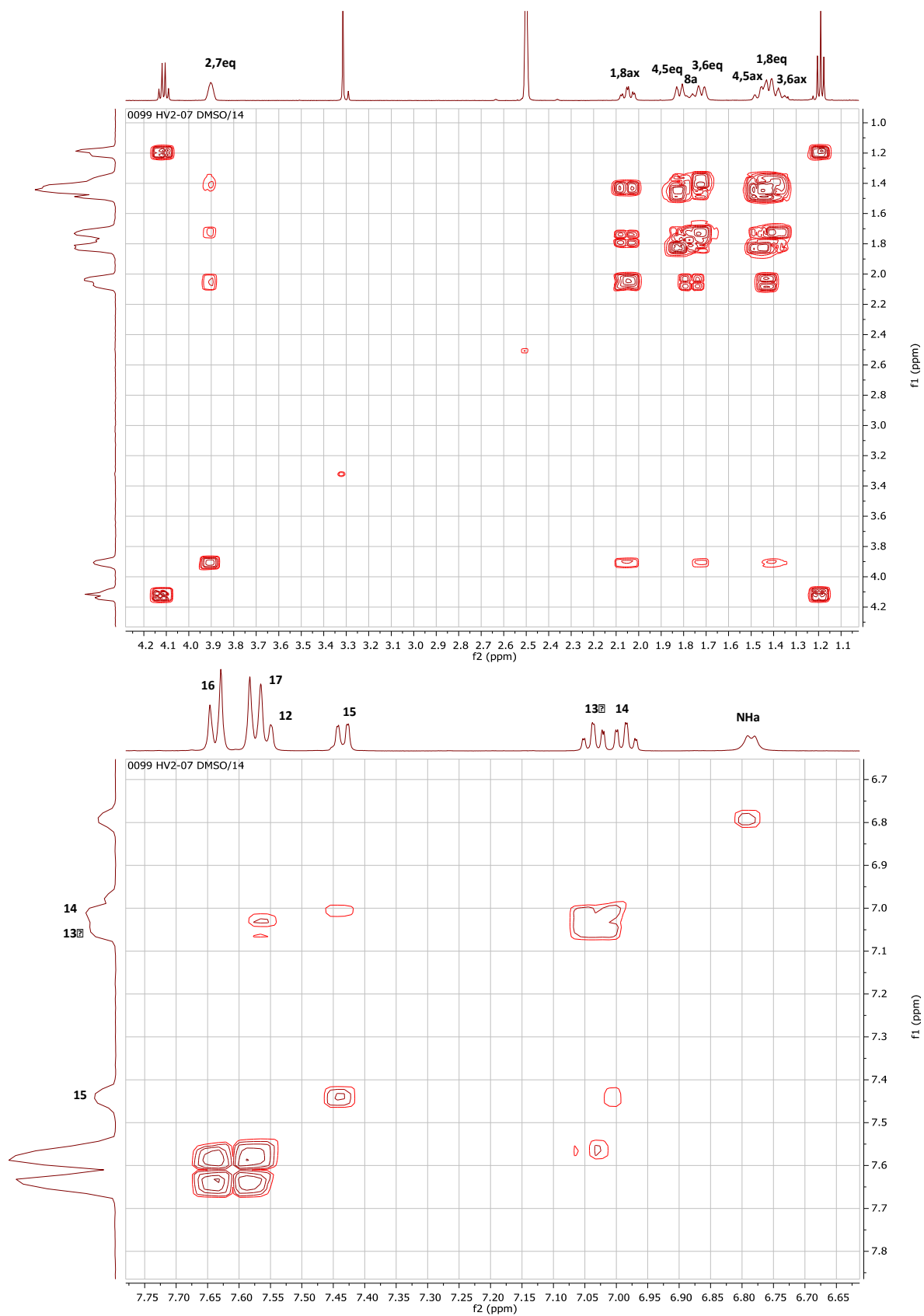


Figure S13. 2D COSY spectra of **7** in DMSO- d_6 (500 MHz).

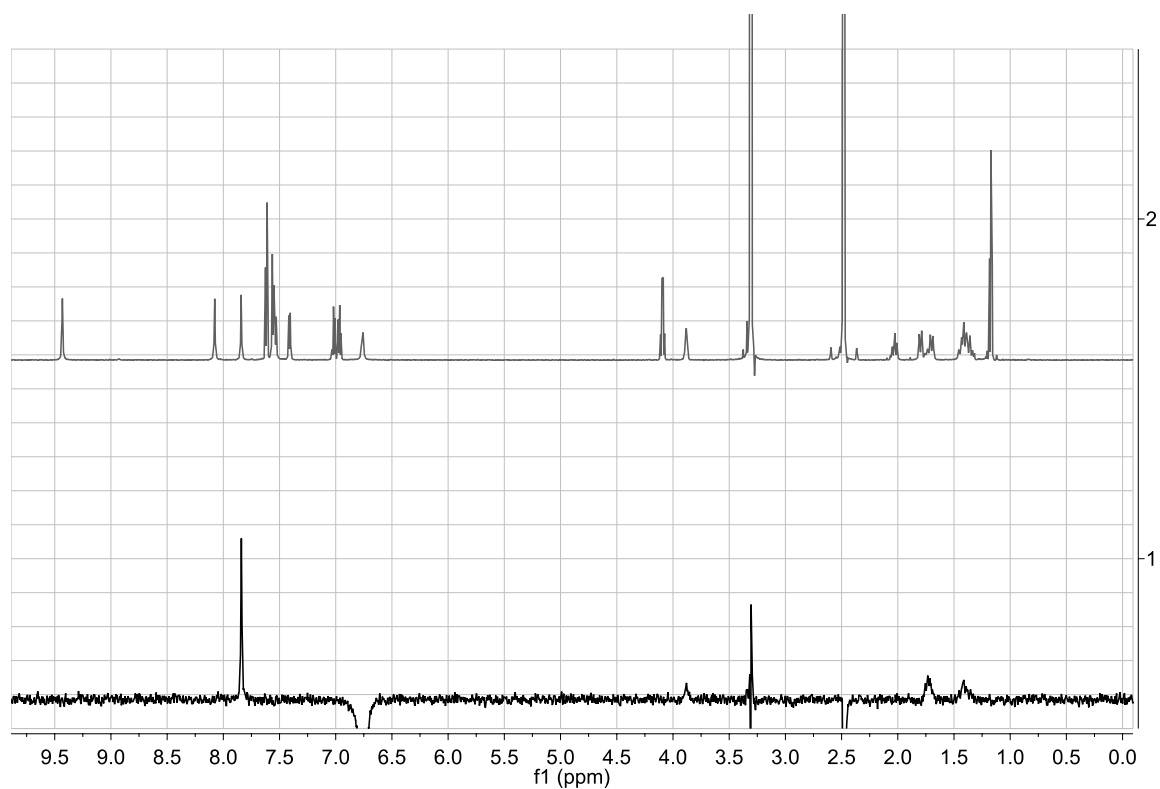


Figure S14. ^1H NMR spectrum of **7** in DMSO-d_6 (top; 600 MHz) and 1D ROESY spectrum of **7** in DMSO-d_6 with NH^a inverted (bottom; 600 MHz).

3. Additional anion transport data and graphs

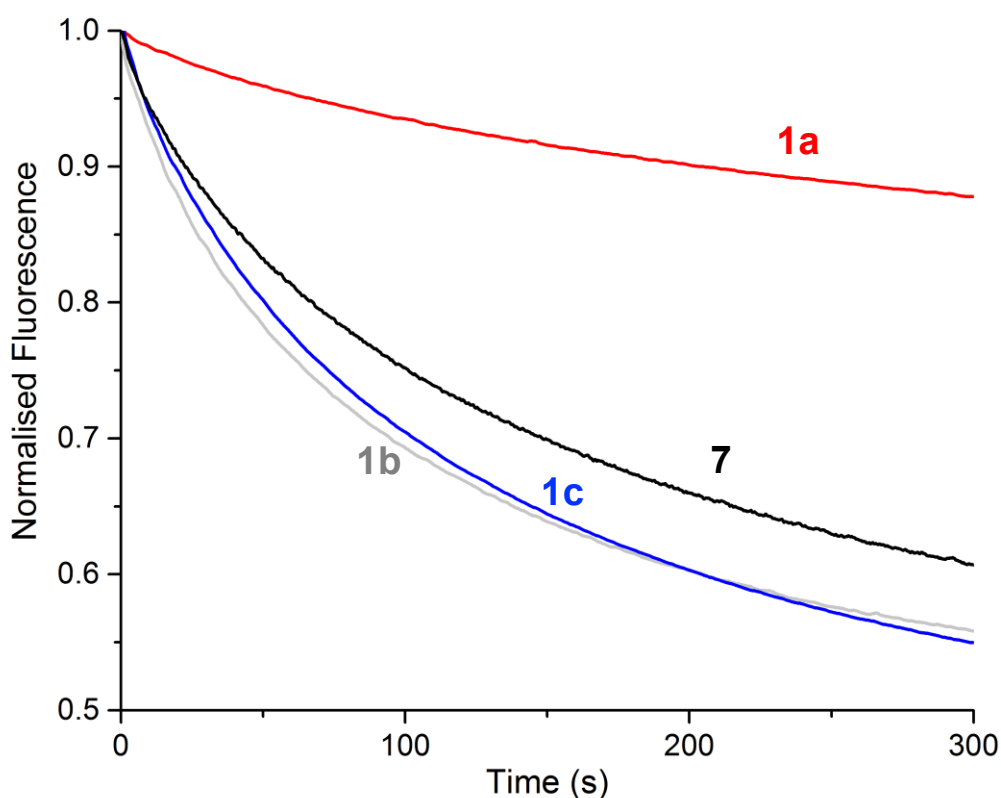
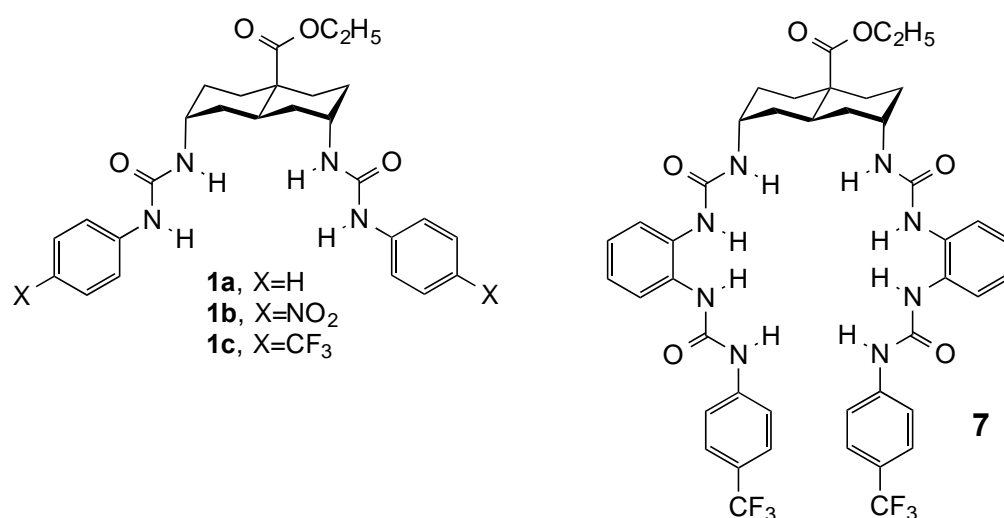


Figure S15. Comparison of the rates of anion transport by **7** with that of previously reported compounds **1a-c**.^{1,2} All compounds were preincorporated at a transporter to lipid ratio of 1:2500 in liposomes composed of POPC and cholesterol (7:3, 0.4 mM total lipid concentration), containing lucigenin. NaNO₃ (225 mM) was present both inside and outside of the liposomes and the transport measurement was initiated by addition of a pulse of NaCl (25 mM).



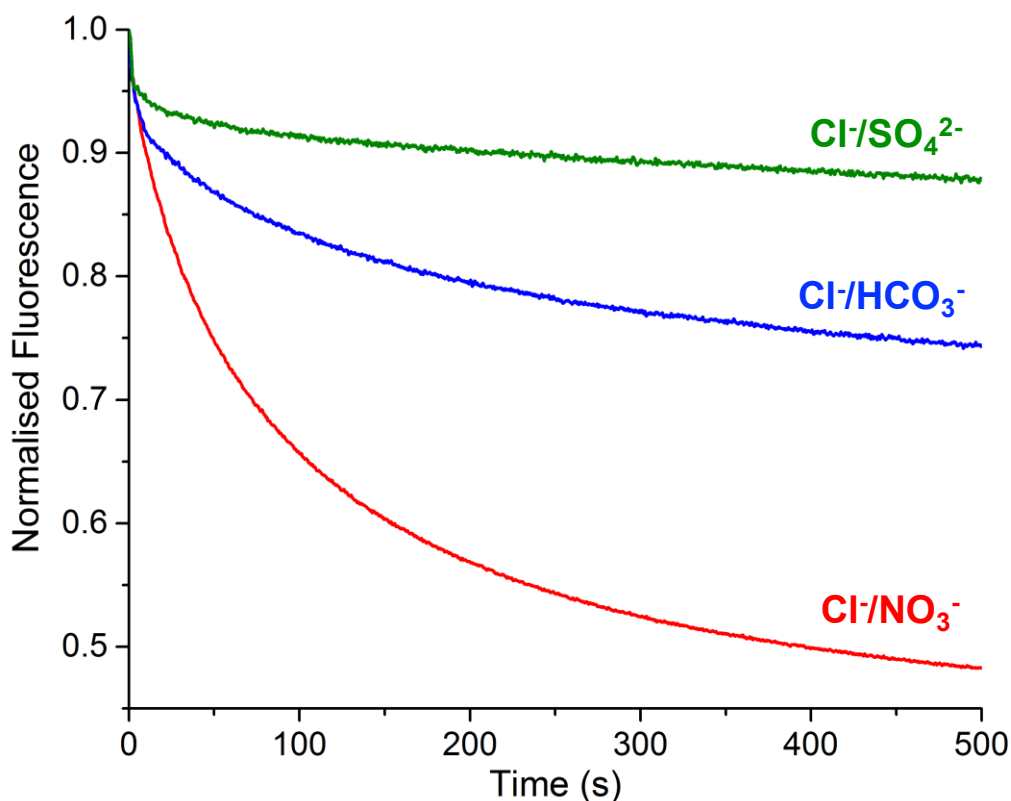


Figure S16. Comparison of the rates of anion transport by **7** in the presence of different anions. Carrier **7** was preincorporated at a transporter to lipid ratio of 1:1000 in liposomes composed of POPC and cholesterol (7:3), containing lucigenin. Either NaNO₃ (225 mM), or NaHCO₃ (225 mM) or K₂SO₄ (225 mM) was present both inside and outside of the liposomes. The observed trends are similar as those previously found for decalin bis-ureas.^{1,3}

References

- ¹ Hussain S, Brotherhood PR, Judd LW, Davis AP. *J Am Chem Soc* 2011;133:1614.
- ² Li H, Valkenier H, Judd LW, Brotherhood PR, Hussain S, Cooper JA, et al. *Nat Chem* 2016;8:24.
- ³ Lisbjerg M, Valkenier H, Jessen BM, Al-Kerdi H, Davis AP, Pittelkow M. *J Am Chem Soc* 2015;137:4948.